NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
JOHN F. KENNEDY SPACE FLIGHT CENTER

LIMITED SOURCE JUSTIFICATION
(For Federal Supply Schedule Orders Exceeding the Simplified Acquisition Threshold)
(FAR 8.405-6(c)(2))

1. This document is a limited source justification for other than full and open competition prepared by the NASA, John F. Kennedy Space Center.

2. The nature and/or description of the action being approved.

The NASA, Materials Science Laboratory (MSL) Chemistry Branch, identifies unknown contamination on flight hardware and ground support equipment as well supports research at Kennedy Space Center. Many times we are call on to support analysis up against hard decision deadlines and launch schedules to provide contamination and failure analysis that may affect the launch or mission.

This justification provides rational for contracting by limited source for the acquisition of an updated state-of- the- art PANalytical x-Ray Diffraction System to accomplish the analytical goals mentioned above. Our current instrument that does this type of analysis at KSC is currently 30 years old (bought in 1985) and has limited capabilities compared with a newer instruments. A newer instrument can run a wide application of experiments configured for Brag-Brentano, parallel beam, transmission and micro spot diffraction collection providing a much lower limit of detection and wider variety of samples that we could do now. The new detector technology can now collect data 100 times faster that our older instrument. Small samples that would take 16 hour long scans can now be collected to 15-30 minutes.

Procurement of this new instrument is part of Materials Science Laboratories (MSL) obsolescence planning to upgrade and replace older instrument so that our analytical capabilities excel to support NASA launch programs and missions.

3. Description of what is being acquired (the supplies or services required to meet the Agency's needs) – including the estimated value and period of performance.

KSC NASA will negotiate with PANalytical for the purchase of x-ray powder diffractometer that can do crystallographic analysis using experiment configuration of Brag-Brentano, transmission, parallel beam and micro spot collection. The total estimated cost of this effort is $. Historically these instruments will last 20-30 years.

The basic instruments functionality includes but not limited to the following:

- High resolution Bragg Brentano optics
- Parallel Beam Optics using a parabolic mirror with parallel plate collimator with diffracted beam monochromator.

- Spinner stage for reflectance and transmission maintaining sample horizontal for both reflectance and transmission experiments
- Micro spot diffraction
    - Micro spot diffraction area mapping optics with optimized 0.1 mm and 0.3 mm point focus mono-capillary with programmable x,y,z stage and video system
- High Speed strip Detector with monochromator
    - Upgradable in future to 2D and 3D imaging Capability
- Programmable slits
- Large specimen stage to hold samples up to 100 mm x 100mm and 5 pound sample
- Copper, Cu x-ray tube rotatable for line and point foci with auto detection
- 15 position sample holder shall be able to upgrade to 45 positions
- Silicon low background holders for a minimum of 12 samples
- Powder sample holders for a minimum of 12 samples
- Transmission sample holders for a minimum of six samples
- High precision machined optics and accessories for rapid experiment reconfiguration within 2 minutes without further alignment
- Cabinet shielding sufficient for hard (Silver) radiation without additional shielding
- Rietveld analysis
- Percent Crystallinity
- Crystallite size/micro-strain
- Inorganic Crystal Structure Database (ICSD) Database with non-expiring license with use up to 10 computers with 161,000 plus reference patterns
- PDF-2
- Computer with 22" monitor and printer

All utilities such as water chiller, air compressor shall be included and no additional facility modifications would be required other than potable water supply and electrical.

Based upon market research of powder diffractometer with commercial sources and interviews with NASA, Air Force Material Centers and University users over the last five years, it has been determined that the PANalytical x-ray powder diffractometer encompasses several unique salient characteristics that are critical to KSC NASA mission. Specific unique, required features provided only by this system are described below.

- Rotation of the x-ray tube to a point source foci for preforming micro beam diffraction, would give maximum (tenfold increase) of x-ray flux over source designs that aperture line source or CBO-f polycapillary optics.

- Manual rotation of the x-ray tube, without disconnecting water and power lines for configuration from line to point focus with auto anode detection of position in less than 5 minutes by inexperienced users without need for realignment of the tube, optics or goniometer manually or via the computer.

- All optical accessories are precision machined to allow rapid experiment design without the need for time consuming realignment. Experiments can be reconfigured in less than 2 minutes by operators at various levels of experiment. This would be a substantial benefit in a multi-user laboratory working with a wide variety of different configurations when dealing with critical support samples. The rapid configuration of the detector and data collection can be done either with or without the monochromator can be done without further alignment.

- A top referencing spinner stage for both reflectance and transmission experiments while maintaining the sample horizontal for both. The instrument, with the auto-sampler will be able to automatically reconfigure to collect sequence samples in both reflectance and transmission without re-alignment or operator intervention.

- A 15 position auto-sampler with the capability to upgrade to a 45 position and a horizontal sample spinner, for both reflectance and transmission experiments, allows for samples to be run consecutively by both techniques for better ability to detect both organic and minor phases.

- High speed pixelated solid state state-of the-art 1D detector with a maximum pixel dimension of 55 micrometers provides the highest resolution for superior peak detection in complex samples where peak overlaps need to be resolved.

- Panalytical provides a 55 micrometer pixel dimension that is included in their 2D and 3D area detectors where the smaller pixel size will be able to detect and resolve overlapping diffraction rings of mixtures.

- Predefined and customizable report generation in a Microsoft Word report format will help export the data directly into our required report formats.

- NASA KSC requires a 72 hour service repair response time due launch support samples. PANalytical can meet this requirement with a local Orlando based service engineer.

- Use of ICSD databases with non-expiring license with use on up to 10 computers for off line data analysis in a multiple user environment. The ICSD database includes 161,000 plus reference patterns.

- Historically KSC has used the Panlytical operating software High Score Plus for a combined 25 years and the training time to master the advanced features capabilities the newer instrument will be minimal.

- The PANalytical data files are in a secure Extensible Markup Language (XML) file format, which is compatible with current historical data collected over the last 15 years and would allow us to continue to evaluate historical data as well corroborate with other NASA Centers and Air Force Logistic Center with the same equipment.

4. Statutory authority permitting other than full and open competition:

This recommendation is made pursuant to FAR 8.405-6 (a)(1)(i)(B) for the acquisition of supplies or services from limited sources under General Services Administration (GSA) Federal Supply Schedules (FSS) when Only one source is capable of providing the supplies or services required at the level of quality required because the supplies or services are unique or highly specialized.

5. A determination by the ordering activity contracting officer that the order represents the best value consistent with 8.404(d).

In accordance with NASA PIC14-01, Class Deviation from FAR 8.404(d), the Contracting Officer will use proposal analysis techniques as descripted in FAR 15.404-1 to determine prices fair and reasonable.

6. A description of the market research conducted among schedule holders and the results or a statement of the reason market research was not conducted.

Panalytical and instruments were evaluated in meeting KSC x-ray powder diffraction needs over the period of the last five years. This involved literature research and interviewing the vendors and current and future instrument users based upon Kennedy Space Center unique analysis and mission requirements, of rapid support analysis with hard deadlines and launch critical samples, as well as supporting current research projects in a multi user environment.

The and X-Ray Diffraction System did not meet the government's minimum requirement. The most significant unique qualities that are needed by the Government that cannot be met by other sources are as following:

The Government has a need for the x-ray source to reconfigure within a 5-min window without any realignment by user support. The ability of the x-ray source to rotate from line to point foci will fully take advantage of the maximum x-ray flux, for greater sensitivity providing a lower limit of detection on smaller samples. Other vendors aperture down or add an additional focusing optic to the line foci and therefore throw away a large amount (>60 percent) of the available energy needed to detect smaller samples.

Precision machined pinned in place optics, with no further alignment for rapid experiment reconfiguration, is critical in saving time and delays in supporting launch critical analysis especially in a multi-user environment. and equipment requires a 30 minute precision alignment or the precision of machined optics that are not of sufficient tolerances and their reconfiguration requires lengthy realignment.

and x-ray diffraction systems do not provide the ability for a 15 position configuration auto-sampler with the capability to upgrade to a 45 position. This capability provides for the unattended operation overnight and on weekends. In addition, the combination of the 15 position sample changer and a horizontal sample spinner, for both reflectance and transmission experiments, allows for samples to be run consecutively by both techniques to better able to detect both organic and minor phases. Both of these experiments can be automatically configured without any user involvement.

7. Any other facts supporting the justification.

As stated above.

8. A statement of the actions, if any, the agency may take to remove or overcome any barriers that led to the restricted consideration before any subsequent acquisition for the supplies or services is made.

The agency continually attempts to overcome barriers to competition by analyzing different sources that might be qualified for similar future acquisitions. However, the unique nature of the Diffraction System does not lend itself this goal due to the critical criteria stated in Section 3 of this document. If the requirement changes, the Agency will begin surveying the market for new sources

Technical Officer:

I certify that the supporting data presented in this justification are accurate and complete.

Philip M. Howard — 23 July 2014
Philip M. Howard (Date)
AST, Structural Materials

Contracting Officer:

I certify that this justification is accurate and complete to the best of my knowledge and belief.

Kelly J. Boos — 7/23/14
Kelly J. Boos (Date)
Contracting Officer